

KnowItAll Software Training

Drawing Structures and Reactions

Drawing Structures and Reactions

How to Use ChemWindow to Create and Edit Structures

Purpose

The ChemWindow application is a full-featured 2-dimensional structure drawing program. You can use the ChemWindow application to create chemical structures that can be used throughout the KnowItAll Informatics System for searching, prediction and reporting chemical composition.

Objectives

This exercise will teach you:

- How to use basic ChemWindow tools to create and edit a structure drawing
 - How to save a structure for further use
 - How to send structure from ChemWindow to MS office documents
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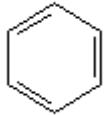

Background

Chemical structures can be used throughout the KnowItAll Informatics System for searching, prediction and reporting chemical composition.

KnowItAll Applications Used

- ChemWindow®

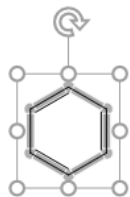
Begin a new structure drawing

	Action	Result
1	Click the ChemWindow icon in the Basics toolbox.	The ChemWindow application opens to a blank drawing pane.
2	Select the Benzene Ring tool  in the Main section of the Chemistry Toolbar .	
3	Move the cursor into the drawing area, then click to draw a benzene ring.	The benzene ring structure is placed in the drawing area. 
4	<p>If desired, use tools on the zoom toolbar to change the magnification.</p> <p>Note: Choose View > Zoom Toolbar to toggle the toolbar display.</p>  <p>The ctrl + scroll function can also be used to zoom in and out quickly.</p>	



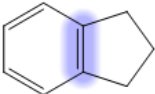



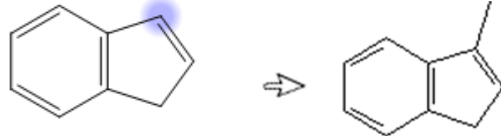
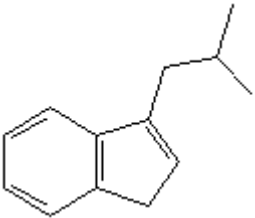
5

Use the **Selection** tool  to select the structure and move it within the workspace.

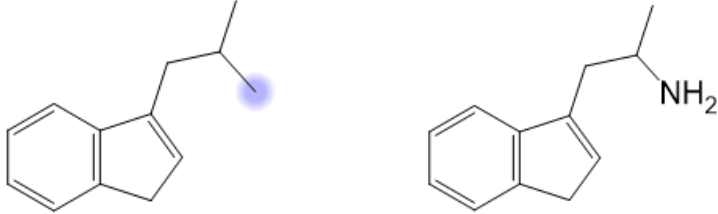
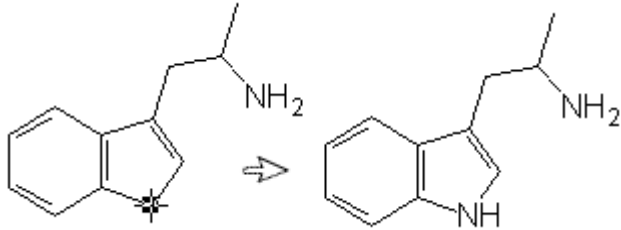
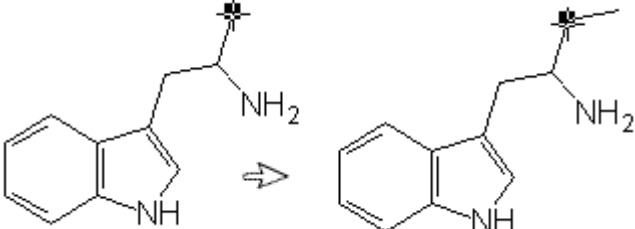
Graphic handles appear when the structure is selected.

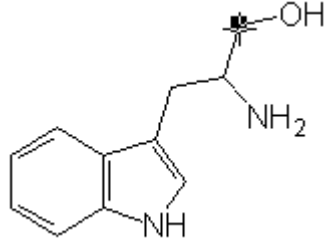
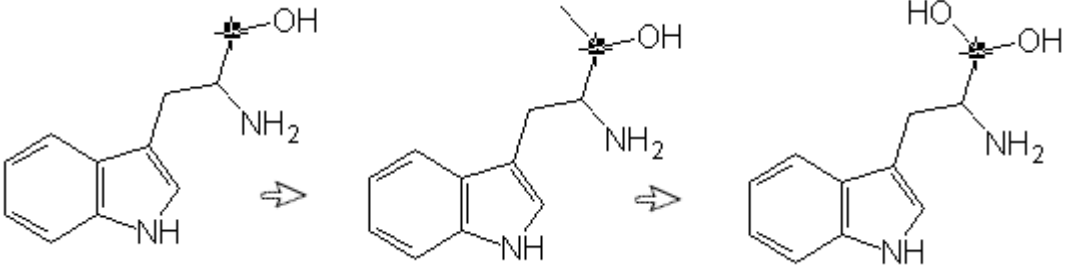
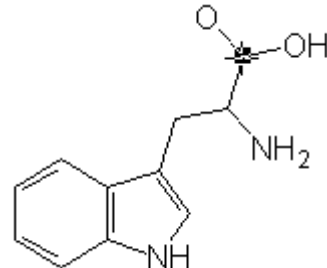


Add features to the structure

	Action	Result
1	Select the Cyclopentane tool  , then move the cursor to the highlighted bond on the benzene ring.	
2	Click to join a cyclopentane ring to the benzene ring.	
3	Open the Bonds group in the Drawing Toolbar and select the Inside Double Bond tool  . Then use it to add a double bond to the structure.	
4	Select the Single Bond tool  . Then move the cursor over the atom's hit box as shown. Click to create a single bond.	 Note: If you don't release the cursor, you can control the bond direction by dragging.
5	Continue adding single bonds by clicking on hit boxes on atoms.	

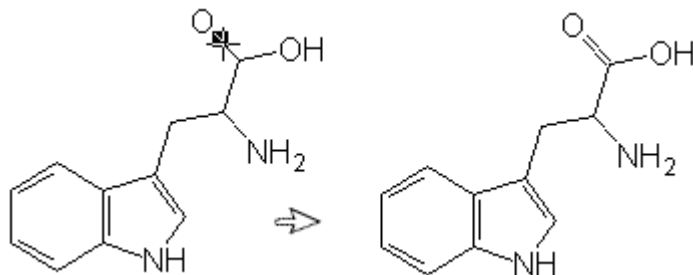
Use hot keys to add nitrogen and oxygen atoms

	Action	Result
1	Move the cursor over the terminal carbon. Then press n on your keyboard.	<p>NH₂ appears at the end of the bond.</p>  <p>>></p> <p>Note: Numbers are automatically displayed as subscripts when using hot keys, which are shortcut keys you can use to quickly label atoms.</p> <p>You can also use the atom label tool to add atoms to a drawing. However, unlike atoms added while using a bond tool, atoms in atom labels are not actually part of the structure and will not be included when calculating the mass or chemical formula.</p>
2	Repeat to replace a carbon atom with NH .	
3	With the single bond tool still selected, place your cursor over the terminal carbon atom and click to add another single bond.	

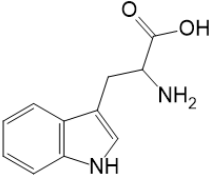
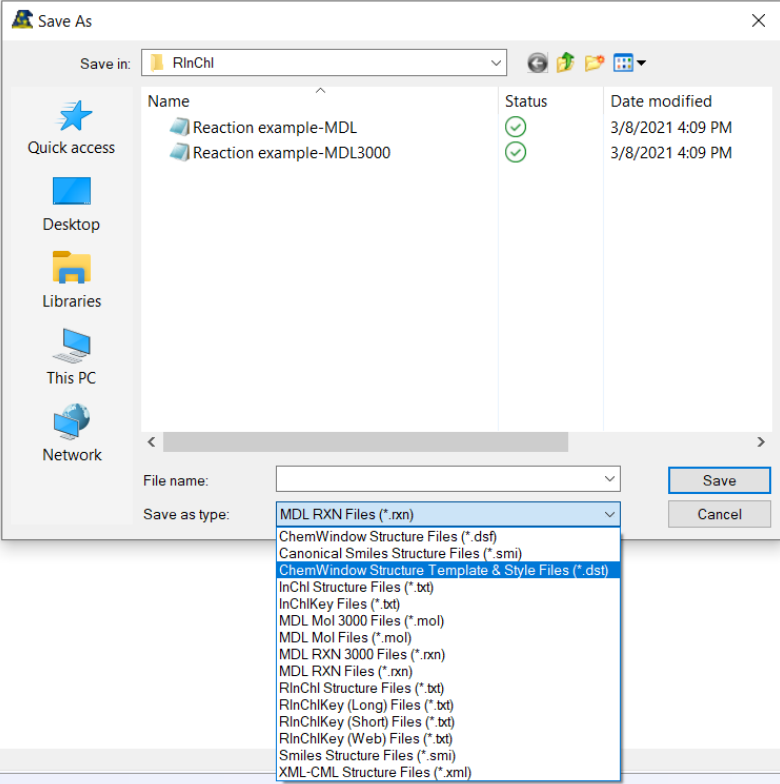
4	Without moving the cursor, press o on your keyboard.	 <p>The diagram shows the chemical structure of tryptamine (2-(2-aminophenylethyl)indole-3-carboxamide). A cursor, represented by a small black square with a crosshair, is positioned on the alpha carbon of the ethyl side chain. This carbon is bonded to a hydrogen atom (not explicitly drawn), a hydroxyl group (-OH), and an amino group (-NH₂).</p>
5	Click to sprout another single bond. Then press o on the keyboard to add a hydroxyl group.	 <p>The diagram illustrates the step-by-step addition of a second hydroxyl group to the alpha carbon. It consists of three chemical structures connected by right-pointing arrows (⇒). 1. The first structure is identical to the one in step 4, with a cursor on the alpha carbon. 2. The second structure shows a single bond sprouting from the alpha carbon, and the cursor has moved to this new bond. 3. The third structure shows a second hydroxyl group (-OH) attached to the alpha carbon, resulting in a geminal diol (1,1-dihydroxy-2-(2-aminophenylethyl)indole-3-carboxamide).</p>
6	Press o again to remove the hydrogen. Note: When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.	 <p>The diagram shows the chemical structure of tryptamine with a cursor on the alpha carbon. A hydrogen atom is being removed from this carbon, as indicated by the note. The structure is identical to the one in step 4, but the note explains that pressing the 'o' key repeatedly will change the number of hydrogens attached to the atom.</p>

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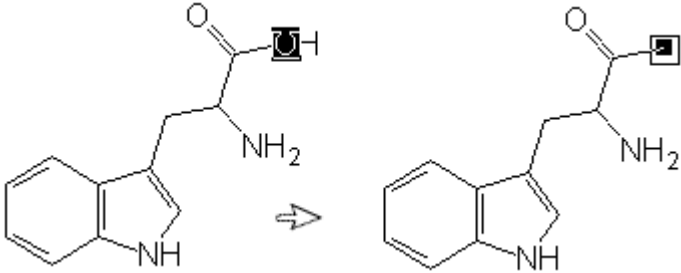
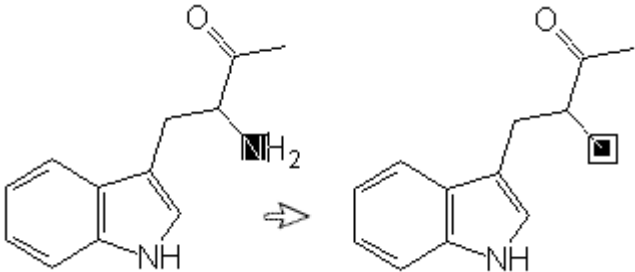

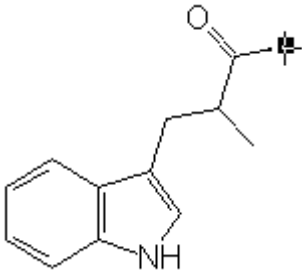
Move the cursor to the hit box on the bond. Then click to create a double bond.

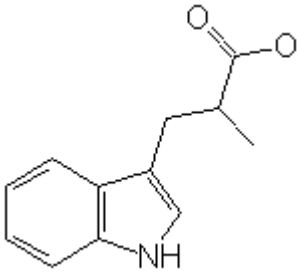


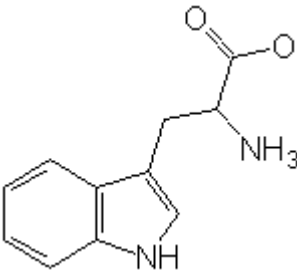

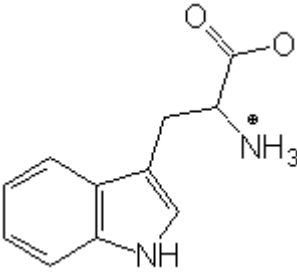



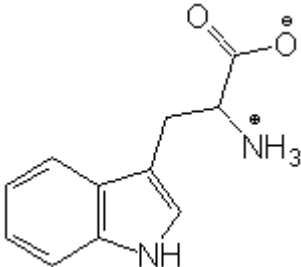
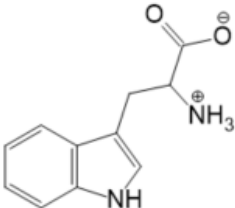

Save the structure

	Action	Result
1	<p>Choose File > Save.</p> <p>Note: You can also click the Save button on the toolbar or press Ctrl+S.</p>	<p>The Save As dialog box opens. The default file type (ChemWindow structure file, *.dsf) is already selected, and will be used for this structure. Other file types include ChemWindow Structure Template & Style (*.dst) and MDL Mol file (*.mol).</p>  
2	<p>Navigate to the folder where you wish to save the structure file, then type in the file name "tryptophan."</p>	
3	<p>Click Save.</p>	<p>The structure is saved, and the file name is displayed on the drawing tab.</p>

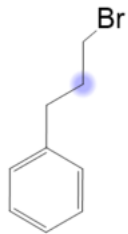
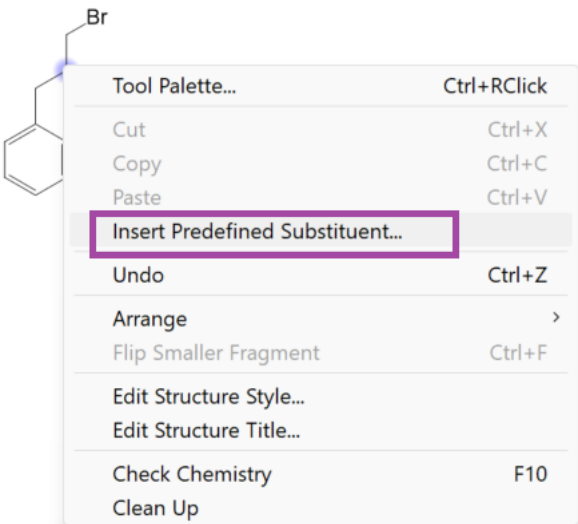
Edit the structure and use atom labels and atom tags

	Action	Result
1	Select the Eraser tool  , then click to remove the hydroxyl.	
2	Click to remove amino groups.	
3	Open the Main group on the Drawing Toolbar and select the Atom Label tool  . Then click where the hydroxyl group was located.	

<p>4</p> <p>Type uppercase O.</p> <p>Note: Atom labels are case-sensitive.</p>	 <p>The image shows a chemical structure of a tryptophan derivative. It consists of an indole ring system (a benzene ring fused to a pyrrole ring) attached to a side chain. The side chain is a 2-amino-3-carboxypropyl group. The carboxylate group is shown as a carbon atom double-bonded to one oxygen atom and single-bonded to another oxygen atom, with a methyl group also attached to the carbon.</p>
<p>5</p> <p>Move to the other atom and type uppercase NH3.</p> <p>Note: Numbers are automatically displayed as subscripts if the Text  is selected.</p> <p>Style toolbar's Formula tool  is selected.</p>	 <p>The image shows the same chemical structure as in row 4, but the carboxylate group has been replaced by an ammonium group. The ammonium group is shown as a carbon atom single-bonded to three hydrogen atoms and one nitrogen atom, with a positive charge symbol (+) above the nitrogen.</p>
<p>6</p> <p>Select the Positive Charge Atom Tag tool  to add a positive charge to the atom.</p>	 <p>The image shows the same chemical structure as in row 5, but the positive charge symbol (+) has been moved from above the nitrogen atom to directly on the nitrogen atom.</p>
<p>TIP</p>	<p>Clicking and dragging a charge allows you more control over the placement of the charge. You can also use the Lasso tool to move the charge.</p>

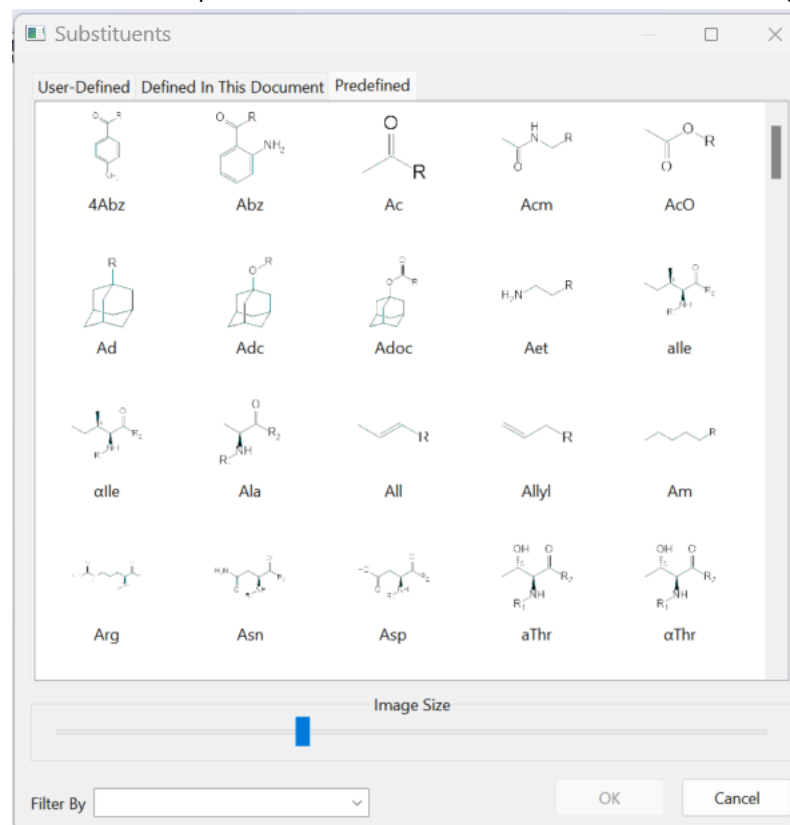
	Action	Result
7	Repeat with the Negative Charge Atom Tag tool  to add a negative charge to the oxygen atom.	
8	Choose File > Save As to save the structure with file name tryptophan2.dsf .	
9	Click the "x" at the bottom tab to close this drawing Click No at saving file prompt This would start a new blank ChemWindow screen.	 

Use pre-defined substituents

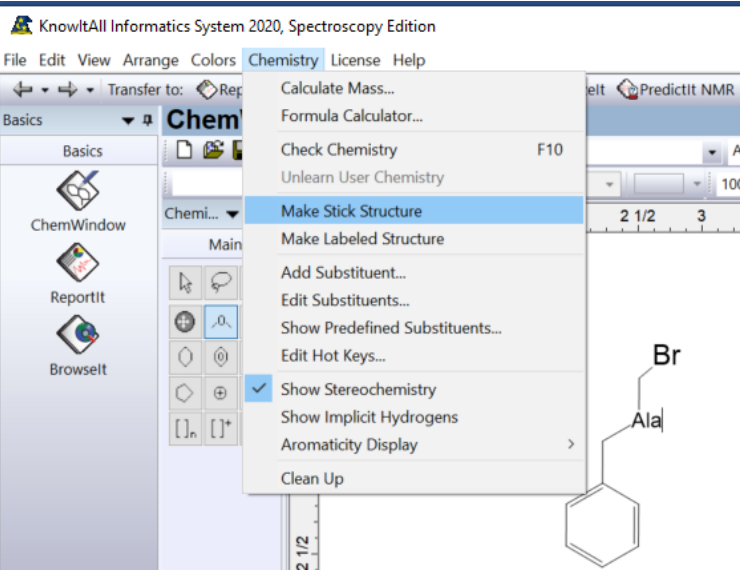
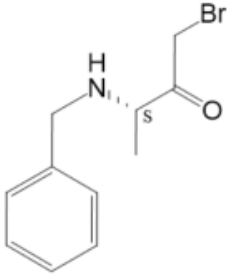
	Action	Result
1	<ul style="list-style-type: none">Draw the structure shownMouse over the atom (it is highlighted)	
2	<ul style="list-style-type: none">Right-mouse-click to bring up menusChoose Insert Pre-defined Substituent	

- 3
- Pick **Ala**
 - **OK**

A table shows all predefined substituents. One can sort the contents using **Filter By**:

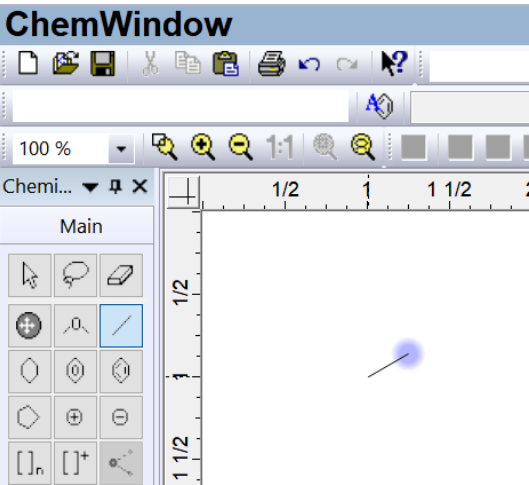
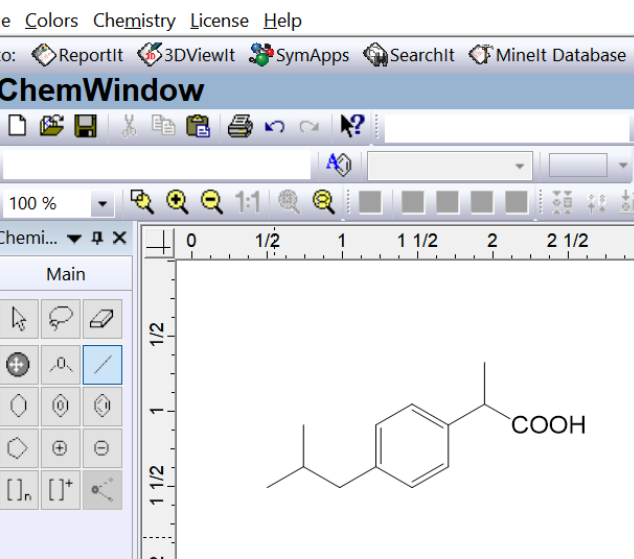


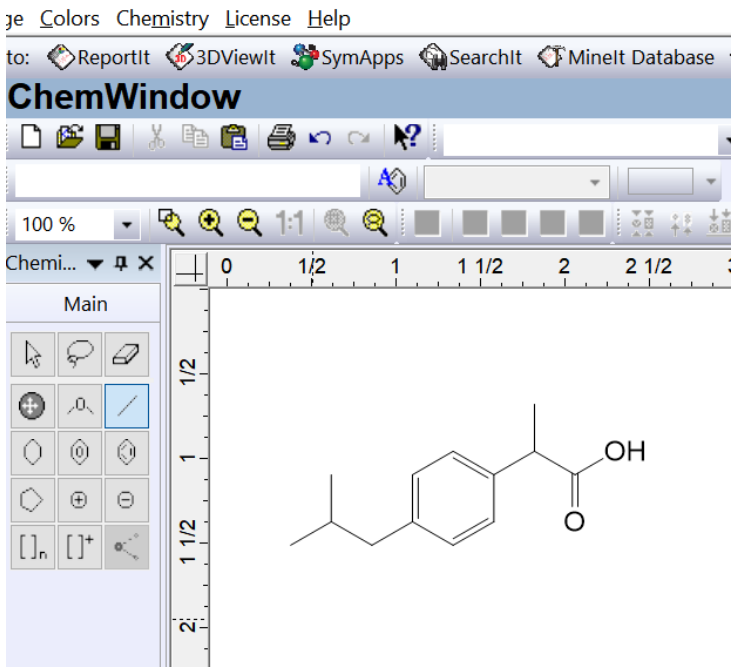
Note: there is another way to achieve this – after one highlights the atom in step 2, one can type in **Ala**, this does require one to know what 3 letters to use.

	Action	Result
4	Click Chemistry > Make Stick Structure .	 <p>KnowItAll Informatics System 2020, Spectroscopy Edition</p> <p>File Edit View Arrange Colors Chemistry License Help</p> <p>Basics</p> <p>Chemistry</p> <ul style="list-style-type: none">Calculate Mass...Formula Calculator...Check Chemistry F10Unlearn User ChemistryMake Stick StructureMake Labeled StructureAdd Substituent...Edit Substituents...Show Predefined Substituents...Edit Hot Keys...<input checked="" type="checkbox"/> Show StereochemistryShow Implicit HydrogensAromaticity DisplayClean Up <p>ChemWindow</p> <p>ReportIt</p> <p>Browselt</p> <p>2 1/2 3</p> <p>2 1/2</p>
5		 <p>The above is the expanded structure.</p>

5	<p>Click the "x" at the bottom tab to close this drawing.</p> <p>Click No at saving file prompt.</p> <p>This would start a new blank ChemWindow screen.</p>	
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Use Hotkeys

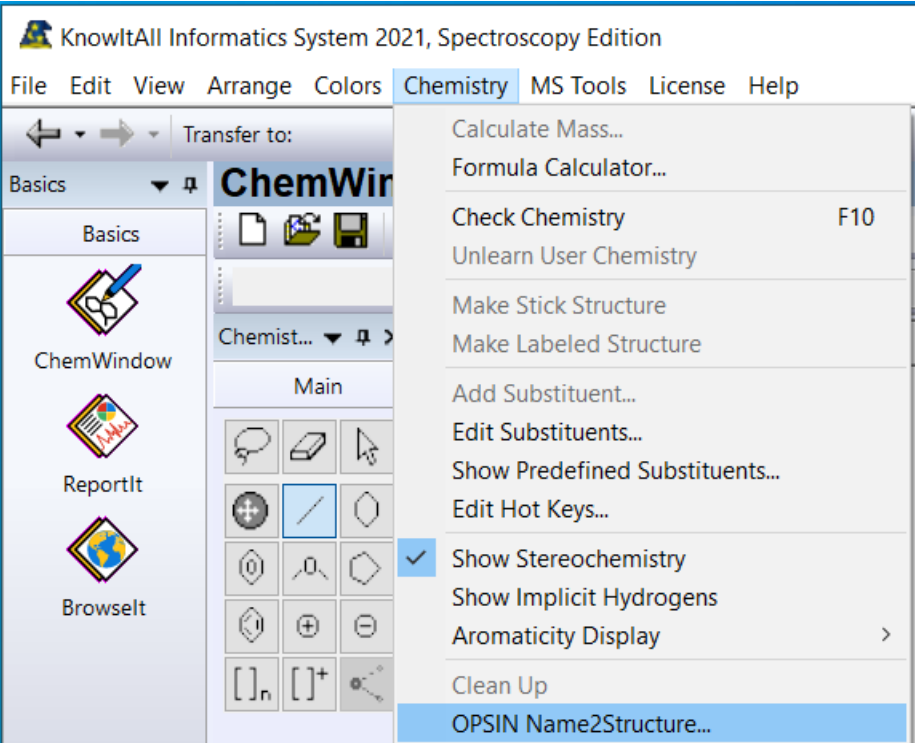
	Action	Result
1	<p>In the Main toolbox, select the Standard bond tool.</p> <p>Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.</p>	
2	<p>Type the following characters on your keyboard: 9, 1, 3, 9, shift + O (Capital letter O).</p> <p>(Note that hot keys involving capital letters use shift + letter, not caps lock + letter.)</p>	

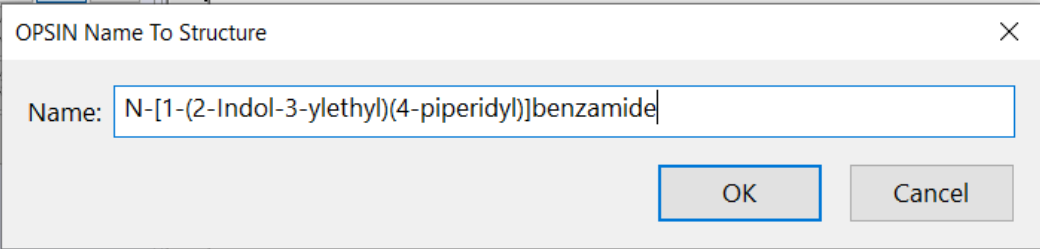
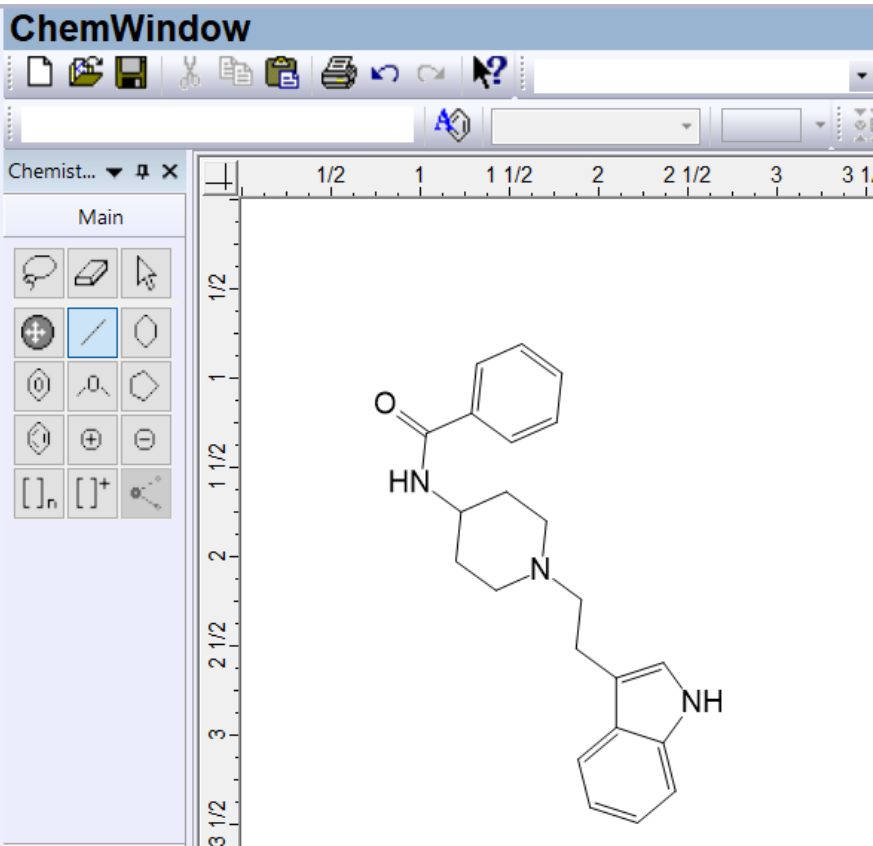
	Action	Result
3	Click Chemistry > Make Stick Structure .	 <p>The above is the expanded structure.</p>
4	Click the "x" at the bottom tab to close this drawing. Click No at saving file prompt. This would start a new blank ChemWindow screen.	

NOTE: You can copy structures and paste to MS office tools. This capability is discussed further in the next session.

Use OPSIN Name2Structure

Example 1 – chemical name

	Action	Result
1	Navigate to Chemistry > OPSIN Name2Structure .	 The screenshot shows the ChemWin software interface. The title bar reads "KnowItAll Informatics System 2021, Spectroscopy Edition". The menu bar includes "File", "Edit", "View", "Arrange", "Colors", "Chemistry", "MS Tools", "License", and "Help". The "Chemistry" menu is open, displaying a list of options: "Calculate Mass...", "Formula Calculator...", "Check Chemistry" (with a keyboard shortcut "F10"), "Unlearn User Chemistry", "Make Stick Structure", "Make Labeled Structure", "Add Substituent...", "Edit Substituents...", "Show Predefined Substituents...", "Edit Hot Keys...", "Show Stereochemistry" (checked), "Show Implicit Hydrogens", "Aromaticity Display" (with a right arrow), "Clean Up", and "OPSIN Name2Structure..." (highlighted in blue). The left sidebar contains icons for "ChemWindow", "ReportIt", and "BrowseIt". The main workspace shows a toolbar with various drawing tools.

2	<p>Enter N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide. Click OK.</p>	
3		<p>The resulting structure is displayed.</p> 

4	<p>Click the "x" at the bottom tab to close this drawing</p> <p>Click No at saving file prompt</p> <p>This would start a new blank ChemWindow screen.</p>	
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Example 2 – common name

Repeat steps 1 – 4, now entering a common name such as cholesterol. **ChemWindow** displays it as a structure.

Drawing Reactions

How to Use ChemWindow to Draw Reactions

Purpose

ChemWindow to create reactions and transfer them to MS tools as well as ReportIt application.

Objectives

This exercise will teach you:

- How to draw chemical reactions
 - How to work with MS office tools
-

Background

Scientists can use the KnowItAll's ChemWindow application to create reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

Training Files Used in This Lesson

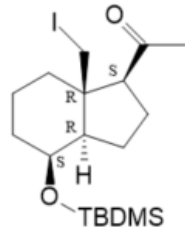
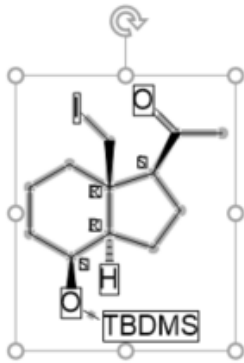
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions


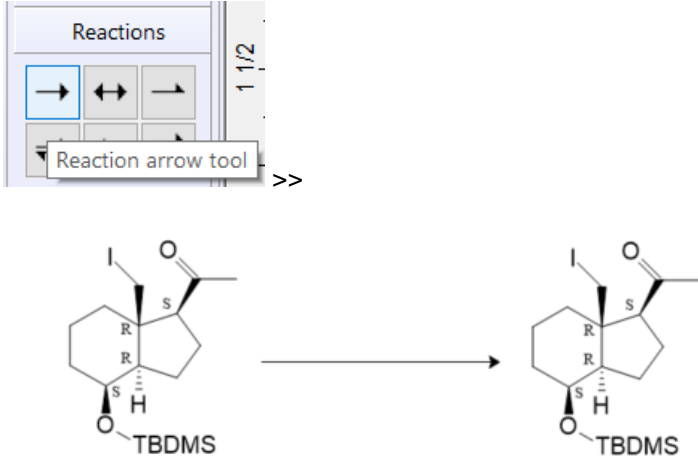
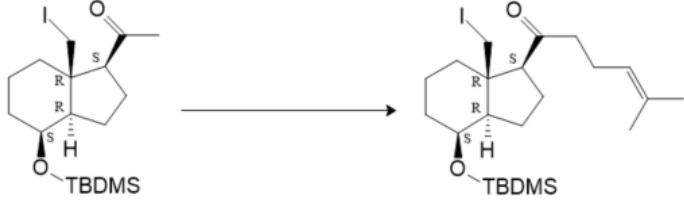
- Reactant.dsf

KnowItAll Applications Used

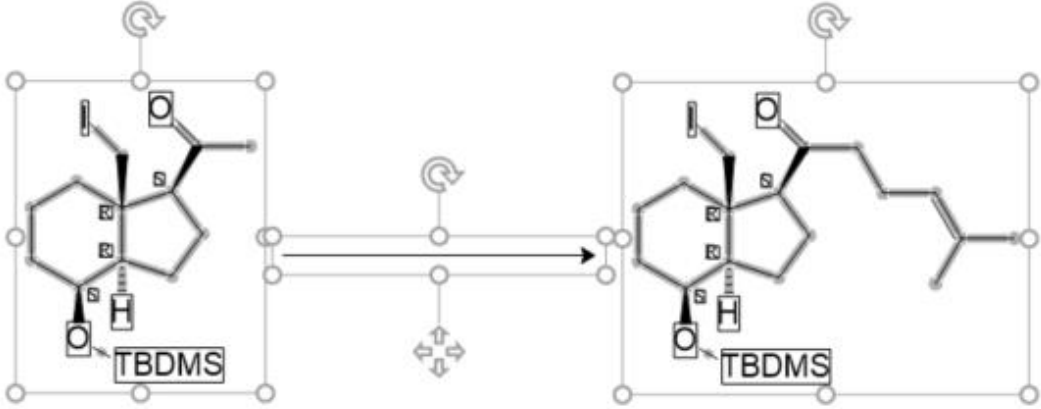
- ChemWindow®

Draw Chemical Reactions

	Action	Result
1	Click the ChemWindow icon in the Basics toolbox.	The ChemWindow application opens to a blank drawing.
2	Navigate to File > Open , then navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions . Select Reactant.dsf . Click Open .	The file opens in the workspace.  <p>The image shows a chemical structure of a bicyclic molecule. It consists of a six-membered ring fused to a five-membered ring. The six-membered ring has an iodine atom (I) attached to one of its carbons. The five-membered ring has a methyl ketone group (C(=O)CH₃) attached to one of its carbons. A hydroxyl group (OH) is attached to the five-membered ring, and the oxygen atom is protected by a tert-butyldimethylsilyl (TBDMS) group.</p>
3	Select the structure.	 <p>The image shows the same chemical structure as in step 2, but it is now enclosed in a selection box. The selection box is a rectangle with small circles at the corners. A rotation handle (a circle with a curved arrow) is visible at the top of the selection box. The TBDMS group is labeled with a box.</p>

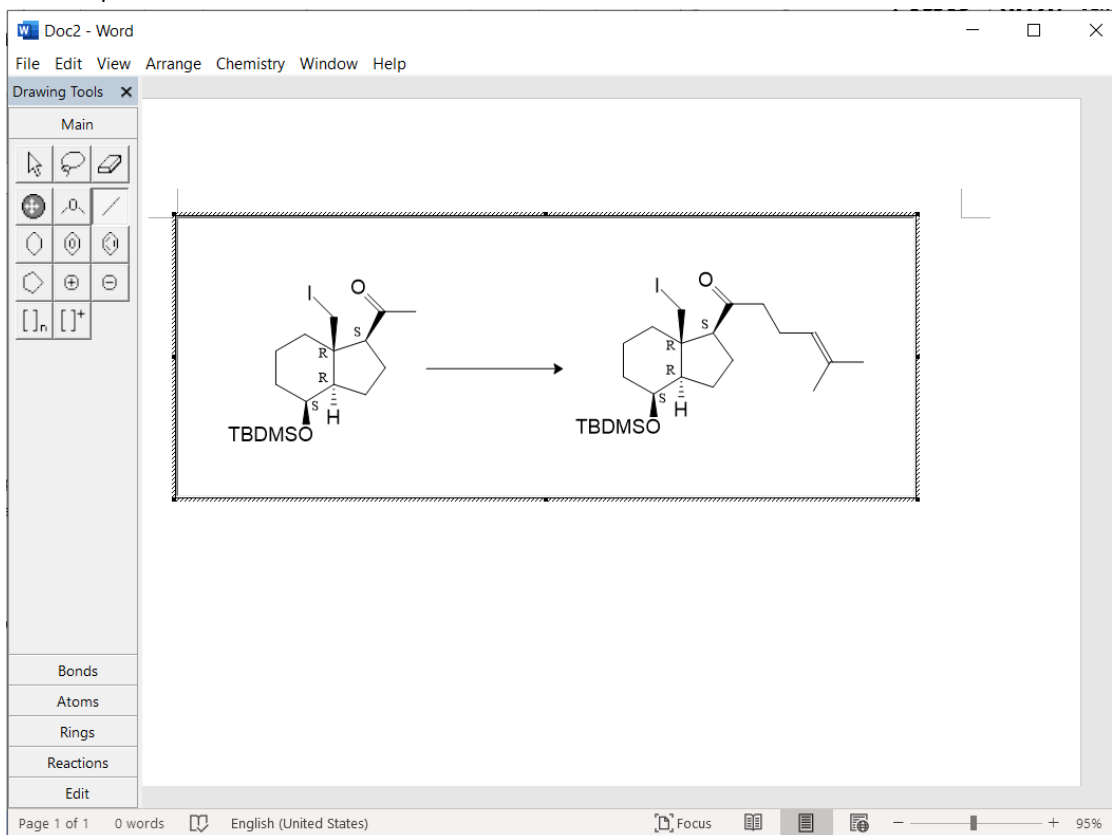
4	Navigate to Edit > Copy , then Edit > Paste .	
5	In the Reactions toolbox, select Reaction arrow tool and draw between the two structures.	
6	Modify the structure on right to be the product.	

OLE connection with MS Office tools

	Action	Result
1	Select the structure object and copy it.	
2	Paste in MS Word. Save the Word document. Close KnowItAll.	

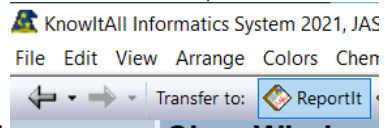
- 3 In the MS Word document, double-click on the KnowItAll object saved.

You can perform ChemWindow actions from here.



TIP: You can work with other MS office tools in the same way.

NOTE: For complex text editing with structure and reactions, we recommend you transfer what is in **ChemWindow** to the **ReportIt** application. You can do this by



using the **Transfer to: ReportIt** function.

Mass Spectrometry Tools

How to Use the Mass Spectrometry Tools in ChemWindow

Purpose

This exercise demonstrates how to use tools specially made for Mass Spectrometry.

Objectives

This exercise will teach you:

- How to calculate Isotopic Distribution for a structure
 - How to calculate elemental composition
 - How to use the MS fragmentation tool
-

Background

Scientists can use the KnowItAll's ChemWindow application to add reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

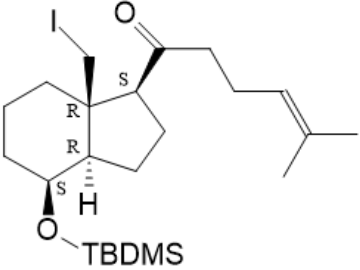
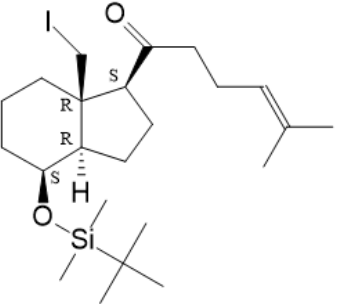
Training Files Used in This Lesson

- Structure 2.dsf

KnowItAll Applications Used

- ChemWindow®

Isotopic Distribution

	Action	Result
1	<p>Navigate to File > Open, then navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions folder.</p> <p>Select Product.dsf.</p> <p>Click Open.</p>	 <p>The chemical structure shows a bicyclic system consisting of a six-membered ring fused to a five-membered ring. The six-membered ring has an iodine atom (I) attached with a wedge bond and a hydrogen atom (H) attached with a dashed bond. The five-membered ring has a ketone group (C=O) attached with a wedge bond and a hydrogen atom (H) attached with a dashed bond. A tert-butyldimethylsilyloxy (TBDMS) group is attached to the oxygen atom of the alcohol group. A side chain is attached to the five-membered ring, consisting of a propyl chain ending in a terminal alkene group with a methyl substituent.</p> <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>Navigate to Chemistry > Make Stick Structure.</p>	 <p>The stick structure shows the same bicyclic compound as in the previous row, but with a more detailed representation of the TBDMS group, showing the silicon atom (Si) and its three methyl groups.</p>

- 3 Navigate to **MS Tools > Calculate Isotopic Distribution**.
- In the pop-up window, click **Calculate**.

KnowItAll Informatics System 2021, Spectroscopy Editor

ChemWindow

Isotopic Distribution Calculator

Chemical Formula: $C_{23}H_{41}IO_2Si$

Calculation Method: Low Resolution

Minimum Intensity: 0.1 %

Peak Table:

Mass	Intensity
------	-----------

Copy Spectrum Copy Peak Calculate Close

TBDMS

4

Isotopic Distribution Calculator

Chemical Formula: $C_{23}H_{41}IO_2Si$

Calculation Method: Low Resolution

Minimum Intensity: 0.1 %

Peak Table:

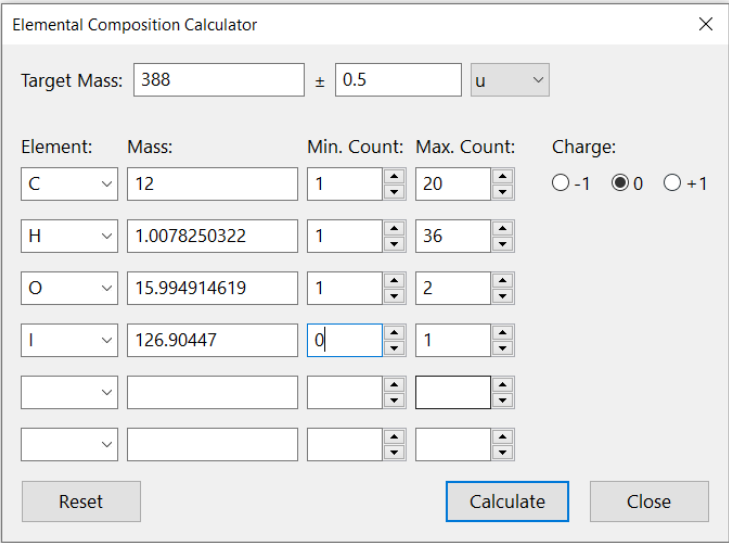
Mass	Intensity
504	100.0000
505	29.9539
506	7.9809
507	1.3092

Copy Spectrum Copy Peak Table Calculate Close

- 5 Close this dialog

Isotopic Elemental Composition

This tool is not associated with a database record structure.

	Action	Results																																			
1	Navigate to MS Tools > Calculate Elemental Composition.	<p>This dialog shows up.</p>  <p>Elemental Composition Calculator</p> <p>Target Mass: 388 ± 0.5 u</p> <table border="1"><thead><tr><th>Element:</th><th>Mass:</th><th>Min. Count:</th><th>Max. Count:</th><th>Charge:</th></tr></thead><tbody><tr><td>C</td><td>12</td><td>1</td><td>20</td><td><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</td></tr><tr><td>H</td><td>1.0078250322</td><td>1</td><td>36</td><td></td></tr><tr><td>O</td><td>15.994914619</td><td>1</td><td>2</td><td></td></tr><tr><td>I</td><td>126.90447</td><td>0</td><td>1</td><td></td></tr><tr><td></td><td></td><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td><td></td><td></td></tr></tbody></table> <p>Reset Calculate Close</p>	Element:	Mass:	Min. Count:	Max. Count:	Charge:	C	12	1	20	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1	H	1.0078250322	1	36		O	15.994914619	1	2		I	126.90447	0	1											
Element:	Mass:	Min. Count:	Max. Count:	Charge:																																	
C	12	1	20	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1																																	
H	1.0078250322	1	36																																		
O	15.994914619	1	2																																		
I	126.90447	0	1																																		

2 Fill in elements and occurrences and click **Calculate**.

Combinations of elements are displayed.

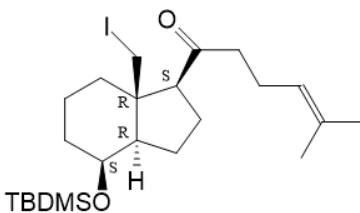
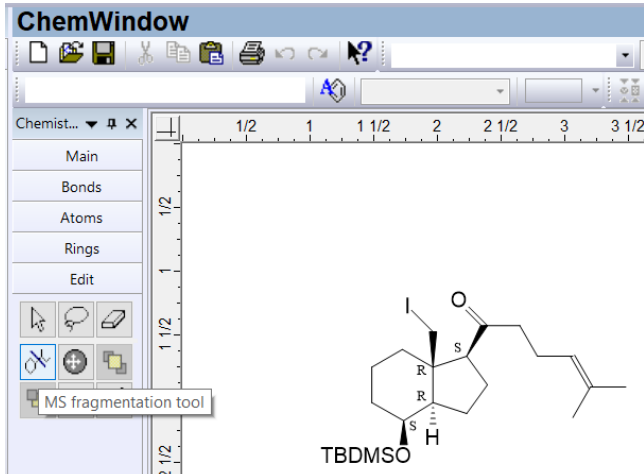
Elemental Composition Results

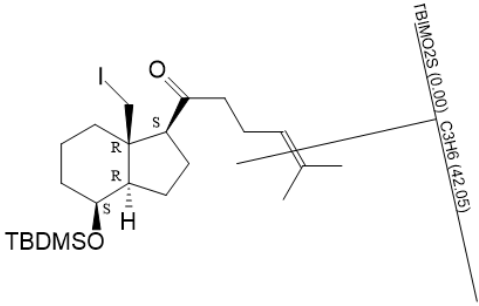
Target Mass: 388 ± 0.5 u
Charge: 0 Result Count: 6

C	H	O	I	m	Δm [u]	Δm [ppm]
18	13	2	1	387.9960	-0.0040	-10.2457
19	17	1	1	388.0324	0.0324	83.5314
20	5	1	1	387.9385	-0.0615	-158.4799
17	25	2	1	388.0899	0.0899	231.7656
19	1	2	1	387.9021	-0.0979	-252.2570
18	29	1	1	388.1263	0.1263	325.5427

Copy To Clipboard Close

MS Fragmentation

	Action	Result
1	<p>Navigate to File > Open. Then navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions folder.</p> <p>Select Product.dsf.</p> <p>Click Open.</p>	 <p>TBDMSO</p> <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>In the Edit toolbox, select the MS fragmentation tool.</p>	 <p>ChemWindow</p> <p>Main Bonds Atoms Rings Edit</p> <p>MS fragmentation tool</p> <p>TBDMSO</p>

3		 <p>The image shows a chemical structure of a bicyclic molecule. It consists of a six-membered ring fused to a five-membered ring. The six-membered ring has an iodine atom (I) on a wedge and a tert-butyldimethylsilyloxy group (TBDMSO) on a dash. The five-membered ring has a carbonyl group (C=O) on a wedge. A separate fragment is shown to the right, consisting of a double bond with two methyl groups and a tert-butyl group. A line connects this fragment to the carbonyl oxygen of the bicyclic molecule. The fragment is labeled with its chemical formula: $\text{TBMOZS (10.00) C}_9\text{H}_{16} \text{ (42.05)}$.</p> <p>You can clip the structure into two fragments.</p>
4	Click Close (X)	